Interaction of electrons with vibrating molecules: molecular electronics applications

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Abstract

Interaction of the electric current, flowing through the molecular junction, with the internal vibrations of the bridging molecule is investigated. Two different theoretical approaches which allow us to calculate the current and other characteristics of the junction are compared. The first method is based on the scattering theory and Landauer formula, and the second on the Wangsness-Bloch-Redfield master equation technique. A set of original models of the molecular bridge with anharmonic vibrational mode and asymmetric coupling to the leads is formulated. Influence of anharmonic vibrations and different types of symmetry in the junction on the current-voltage dependencies of the bridge are discussed. As an example of the phenomenon, which can only be found beyond the harmonic approximation, we demonstrate the existence of the so called "motor effect", i. e. the strong dependence of the average angular momentum of the molecule on the voltage, applied across the junction. The key parameters, responsible for the effect appearance, such as the rotational barrier height and the symmetry in the junction are discussed.